

## Curriculum Vitae (CV)

**Name:** Jianmin Tao

**Current Position:** Director's Postdoctoral Fellow

**Immigration Status:** U.S. Permanent Residency

T-CNLS, MS B258

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### Objective:

- (1) Development of the static and time-dependent density functionals for electronic structure calculations of molecules, solids, and surfaces;
- (2) Application of the static and time-dependent density functional theories to molecules and solids;
- (3) Teaching physics or chemistry courses as a faculty member at research universities.

### Research Interests:

- 1) Time-dependent density functional theory (TDDFT):
  - (i) Construction of dynamical exchange-correlation potentials;
  - (ii) Continuum mechanics for nanoscale systems.
- 2) Theory of ultrafast optical phenomena for strongly correlated electronic materials.
- 3) Density functional theory (DFT):
  - (i) Development of self-interaction corrected functionals;
  - (ii) Long-range van der Waals interaction correction;
  - (iii) Meta-generalized gradient approximations;
  - (iv) Construction of the exchange-correlation hole.
- 4) Current-density functional theory:

Construction of current-density functionals for systems in a magnetic field.
- 5) Application of TDDFT/DFT to nanoscale systems.

### Educational Background:

- 1/1998–5/2002 Ph.D degree in Physics with GPA = 3.9/4, Tulane University, New Orleans, Louisiana  
Dissertation Title: "Density Functional Theory of Atoms, Molecules and Solids: Construction of Accurate Meta-Generalized Gradient Approximations for Exchange and Correlation"  
Dissertation Advisor: Professor John P. Perdew
- 7/1985–1/1988 M.Sc. degree in Chemical Physics, University of Science and Technology of China, Hefei, Anhui, China

Thesis: “Bounds and their applications to atoms and molecules”

Thesis Advisor: Professor Jianmin Li

9/1978–7/1982 B.Sc. in Chemistry, Yunnan Normal University, Kunming, Yunnan, China

### **Professional Experience**

8/2007–present Director’s Postdoctoral Fellow with Dr. Jian-Xin Zhu/T-11 (Strongly Correlated Electron Physics) and Dr. Sergei Tretiak/T-12 (Theoretical Chemistry), Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545. Working on ultrafast optical phenomena in strongly correlated electron materials and application of DFT/TDDFT to the electronic properties of nanoscale systems.

7/2005–7/2007 Postdoctoral Fellow with Professor Giovanni Vignale, Department of Physics, University of Missouri, Columbia, Missouri 65211. Working on time-dependent density functional theory.

6/2002–6/2005 Postdoctoral Fellow with Professor John P. Perdew. Working on the development of density functional theory.

6/2004–12/2004 Adjunct Professor of Physics, Department of Physics, Tualne University. Teaching the calculus-based physics for engineering and science students.

1997–1998 Associate Professor of Chemistry, Yunnan Normal University, Kunming, Yunnan, China. Teaching physical chemistry.

1988–1997 Assistant Professor of Chemistry, Yunnan Normal University, Kunming, Yunnan, China. Teaching physical chemistry.

1982–1985 Teaching Assistant of Chemistry, Yunnan Normal University, Kunming, Yunnan, China. Teaching inorganic chemistry lab.

### **Competitive Honors/Awards:**

2002 Award of the Natural Sciences of Yunnan Province, Yunnan, China

1999 Award for the excellent academic work and research achievement awarded by the educational committee of Yunnan Province, China

1999 Award for excellent papers awarded by Yunnan Normal University, China

Who’s Who in the World (16th edition, 1999)

Who’s Who in America (2009)

### **Relevant Extracurricular Activities:**

Referee papers for

Physical Review Letters

Physical Review B

Journal of Chemical Physics

Journal of Chemical Theory and Computation

International Journal of Quantum Chemistry

Langmuir

Proceedings of the Royal Society A

### Invited Presentations

1. **J. Tao**, van der Waals-Corrected Density Functional Theory, Workshop on Mathematical and Algorithmic Challenges in Electronic Structure Theory, Minneapolis campus of the University of Minnesota, September 29-October 3, 2008.
2. **J. Tao**, Density Functional Theory and Its Time-Dependent Extension, College of Chemistry and Chemical Engineering, Yunnan University, Kunming, P.R. China, June 13, 2008.
3. **J. Tao**, Density Functional Theory and Its Time-Dependent Extension, College of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming, P.R. China, June 12, 2008.
4. **J. Tao**, Density Functional Theory and Its Time-Dependent Extension, Strongly Correlated Electron Physics/T-11, Los Alamos National Laboratory, Los Alamos, New Mexico, October 15, 2007.
5. **J. Tao**, Density Functional Theory and Its Time-Dependent Extension, Department of Physics and Astronomy, University of Louisville, Louisville, Kentucky, January 25, 2007.
6. **J. Tao**, Time-Dependent Density Functional Theory beyond the Local Density Approximation, First LLNL International Symposium and Workshop on Correlated Electrons in Matter, December 8–11, 2006, Half Moon Bay, California.
7. J.P. Perdew, V.N. Staroverov, G.E. Scuseria, and J. Tao, Exact Exchange as a Component of Density Functional Approximations, 231th ACS National Meeting, March 26–30, 2006, Atlanta.
8. **J. Tao**, Density Functionals That Work, Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri, September 21, 2005.
9. **J. Tao**, Nonempirical Construction of a Meta-GGA Density Functional and Useful Extensions, the INT DFT workshop on “Towards a Universal Density Functional for the Nucleus” organized at the Institute for Nuclear Theory in Seattle, September 26-30, 2005.
10. **J. Tao**, Construction and Performance of a Nonempirical Density Functional, Department of Physics and Astronomy, Rutgers The State University of New Jersey, Piscataway, New Jersey, April 14, 2005.
11. **J. Tao**, Meta-Generalized Gradient Approximation: Construction and Performance of a Nonempirical Density Functional, The Third International Workshop on *Electron Correlation and Materials Properties*, Kos, Greece, July 5–9, 2004.

### Grants

2002–2004      Basic And Applied Science Foundation Of Yunnan Province,

	35,000 RMB (1 USD $\approx$ 7 RMB).
1998–2000	National Science Foundation Of China, 74,000 RMB; Basic And Applied Science Foundation Of Yunnan Province, 35,000 RMB; Teaching And Research Foundation Of Yunnan Normal University, 30,000 RMB
1993–1995	Education Foundation Of Yunnan Province, 15,000 RMB

#### Professional Associations:

Member of the American Physical Society (APS)

#### Publications:

##### (i) Submitted and to be submitted

1. **J. Tao**, Density Matrix Expansion and Meta-Generalized Gradient Approximation for the Exchange Energy, to be submitted.
2. **J. Tao** and G. Vignale, Continuum Mechanics of the Inhomogeneous Electron Liquid, to be submitted.
3. **J. Tao**, G. Vignale, and Jian-Xin Zhu, Exchange-correlation stress tensor of the homogeneous system, to be submitted.
4. **J. Tao**, van der Waals interaction-corrected density functional theory, to be submitted.
5. **J. Tao**, Absorption spectra of new blue-light emitting oligoquinolines bearing pyrenyl and triphenyl endgroups from time-dependent density functional theory, submitted.

##### (ii) Peer reviewed

1. J.P. Perdew, V.N. Staroverov, **J. Tao**, and G.E. Scuseria, Density functional with full exact exchange: balanced nonlocality of correlation, and constraint satisfaction, *Phys. Rev. A* **78**: 052513, 2008.
2. **J. Tao**, S. Tretiak, and J.-X. Zhu, Absorption spectra of blue-light emitting oligoquinolines from time-dependent density functional theory, *J. Phys. Chem. B* **112**: 13701, 2008.
3. **J. Tao**, J.P. Perdew, L.M. Almeida, C. Fiolhais, and S. Kümmel, Nonempirical Density Functionals Investigated for Jellium: Spin-Polarized Surfaces, Spherical Clusters, and Bulk Linear Response, *Phys. Rev. B* **77**: 245107, 2008.
4. **J. Tao**, G. Vignale, and I.V. Tokatly, Quantum Stress Focusing in Descriptive Chemistry, *Phys. Rev. Lett.* **100**: 206405, 2008.
5. **J. Tao**, S. Tretiak, and J.-X. Zhu, Excitation energies from a time-dependent nonempirical density functional, *J. Chem. Phys.* **128**: 084110, 2008.
6. **J. Tao**, J.P. Perdew, V.N. Staroverov, and G.E. Scuseria, Exact-exchange energy density in the gauge of a semilocal density functional approximation, *Phys. Rev.*

- A 77*: 012509, 2008.
7. **J. Tao**, G. Vignale, and I.V. Tokatly, Time-dependent density functional theory: Derivation of gradient-corrected dynamical exchange-correlational potentials, *Phys. Rev. B* **76**: 195126, 2007.
  8. J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, V.N. Staroverov, and **J. Tao**, Exact-Exchange Functional Theory for Open Systems of Fluctuating Electron Number, *Phys. Rev. A* **76**: 040501(R), 2007.
  9. J.P. Perdew, A. Ruzsinszky, **J. Tao**, G.I. Csonka, and G.E. Scuseria, One-parameter optimization of a nonempirical meta-generalized gradient approximation for the exchange-correlation energy, *Phys. Rev. A* **76**: 042506, 2007.
  10. **J. Tao**, J.P. Perdew, A. Ruzsinszky, G.E. Scuseria, G.I. Csonka, and V.N. Staroverov, Meta-generalized gradient approximation: Construction and performance of a nonempirical density functional, *Phil. Mag.* **87**: 1071, 2007.
  11. **J. Tao** and G. Vignale, Analytic expression for the diamagnetic susceptibility of a uniform electron gas, *Phys. Rev. B* **74**: 193108, 2006.
  12. **J. Tao** and G. Vignale, Time-dependent density functional theory beyond the local density approximation, *Phys. Rev. Lett.* **97**: 036403, 2006.
  13. L.A. Constantin, J.P. Perdew, and **J. Tao**, Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy, *Phys. Rev. B* **73**: 205104, 2006.
  14. **J. Tao** and J.P. Perdew, Nonempirical construction of current-density functionals from conventional density functional approximations, *Phys. Rev. Lett.* **95**: 196403, 2005.
  15. J.P. Perdew, A. Ruzsinszky, **J. Tao**, V.N. Staroverov, G.E. Scuseria, and G.I. Csonka, Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits, *J. Chem. Phys.* **123**: 062201, 2005.
  16. **J. Tao**, Explicit inclusion of paramagnetic current density in the exchange-correlation functionals of current-density functional theory, *Phys. Rev. B* **71**: 205107, 2005.
  17. **J. Tao** and J.P. Perdew, Test of a nonempirical density functional: Short-range part of the van der Waals interaction in rare-gas dimers, *J. Chem. Phys.* **122**: 114102, 2005.
  18. G.I. Csonka, A. Ruzsinszky, **J. Tao**, and J.P. Perdew, Energies of Organic Molecules and Atoms in Density Functional Theory, *Int. J. Quantum. Chem.* **101**: 506, 2005.
  19. V.N. Staroverov, G.E. Scuseria, J.P. Perdew, **J. Tao**, and E.R. Davidson, Energies of isoelectronic atomic ions from a successful meta-generalized gradient approximation and other density functionals, *Phys. Rev. A* **70**: 012502, 2004.
  20. J.P. Perdew, **J. Tao**, V.N. Staroverov, and G.E. Scuseria, Meta-Generalized Gra-

- dient Approximation: Explanation of a Realistic Nonempirical Density Functional, *J. Chem. Phys.* **120**: 6898, 2004.
21. V.N. Staroverov, G.E. Scuseria, **J. Tao**, and J.P. Perdew, Tests of a Ladder of Density Functional Approximations for Bulk Solids and Surfaces, *Phys. Rev. B* **69**: 075102, 2004.
  22. V.N. Staroverov, G.E. Scuseria, **J. Tao**, and J.P. Perdew, Comparative assessment of a new nonempirical meta-GGA density functional: Molecules and hydrogen-bonded complexes, *J. Chem. Phys.* **119**: 12129, 2003; *ibid.* **121**: 11507(E), 2004.
  23. J.P. Perdew, **J. Tao**, and R. Armiento, How to Tell an Atom From an Electron Gas: A Semi-Local Index of Density Inhomogeneity, *Acta Univ. Debreceniensis de Ludovico Kossuth Nominatae Series Physica et Chimica* **36**: 25, 2003.
  24. **J. Tao**, J.P. Perdew, V.N. Staroverov, and G.E. Scuseria, Climbing the Density Functional Ladder: Non-Empirical Meta-Generalized Gradient Approximation Designed for Molecules and Solids, *Phys. Rev. Lett.* **91**: 146401, 2003.
  25. **J. Tao**, M. Springborg, and J.P. Perdew, Properties of the exchange hole under an appropriate coordinate transformation, *J. Chem. Phys.* **119**: 6457, 2003.
  26. G. Tian, G. Li, and **J. Tao**, Study of Relations between Position and Momentum Expectation Values for Molecules, *Physica Scripta* **66**: 449, 2002.
  27. **J. Tao**, An accurate MGGA-based hybrid exchange-correlation functional, *J. Chem. Phys.* **116**: 2335, 2002; *ibid.* **116**: 10557(E), 2002.
  28. **J. Tao**, Exchange energy density of an atom as a functional of the electron density, *J. Chem. Phys.* **115**: 3519, 2001.
  29. **J. Tao**, P. Gori-Giorgi, J. P. Perdew, and R. McWeeny, Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations, *Phys. Rev. A* **63**: 032513, 2001.
  30. K. Schmidt, S. Kurth, **J. Tao**, and J. P. Perdew, comment on “Correlation holes in a spin-polarized dense electron gas”, *Phys. Rev. B* **62**: 2227, 2000.
  31. P. Ziesche, **J. Tao**, M. Seidl, and J. P. Perdew, How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions, *Int. J. Quantum. Chem.* **77**: 819, 2000.
  32. **J. Tao** and G. Li, Approximate Bounds to the average electron density for atomic systems, *Physica Scripta* **58**: 193, 1998.
  33. **J. Tao**, G. Li, and J. Li, Relationships between radial and momentum expectation values of atoms within the Hartree-Fock approximation, *J. Phys. B: At. Mol. Opt. Phys.* **31**: 1897, 1998.
  34. **J. Tao** and G. Li, Upper bounds for the zeroth-order exchange-energy functional, *J. Phys. B: At. Mol. Opt. Phys.* **31**: 1865, 1998.
  35. **J. Tao**, G. Li, and J. Li, Bounds to information entropies for atomic systems, *J. Chem. Phys.* **107**: 1227, 1997.

36. **J. Tao** and G. Li, Relationships between the zeroth-order kinetic and exchange-energy functionals and the average electron density, *Physica Scripta* 56: 430, 1997.
37. **J. Tao**, G. Li, and J. Li, Rigorous bounds to information entropies for atomic systems, *Physica Scripta* 56: 284, 1997.
38. **J. Tao** and G. Li, Bounds for the zeroth-order exchange-energy functional for atomic systems, *J. Chem. Phys.* 105: 10493, 1996.
39. **J. Tao** and J. Li, Lower bounds to the second-order gradient corrections in the gradient expansions of the kinetic- and exchange-energy functionals for atoms, *Phys. Rev. A* 54: 3859, 1996.
40. **J. Tao**, G. Li, and J. Li, A simple relationship between the second-order gradient correction to the exchange-energy functional and the average electron density for atomic systems, *J. Chem. Phys.* 105: 6995, 1996.
41. **J. Tao** and J. Li, Rigorous lower bounds to the second-order gradient corrections in the gradient expansion of the kinetic and exchange-energy functionals, *Physica Scripta* 54: 337, 1996.
42. **J. Tao** and J. Li, A simple upper bound to electron momentum density, *Physica Scripta* 54: 335, 1996.

**(iii) Not peer reviewed**

1. J.P. Perdew, **J. Tao**, and S. Kümmel, Uniform density limit of exchange-correlation energy functionals in *Recent Advances in Electron Correlation Methodology*, edited by A.K. Wilson and K.A. Peterson (ACS Books, 2007, ACS Symposium Series 958, distributed by Oxford University Press).
2. **J. Tao** and J. P. Perdew, Correlation energy densities: E pluribus unum in *Reviews in Modern Quantum Chemistry: A Celebration of the Contributions of R.G. Parr*, edited by K. D. Sen (World Scientific, Singapore, 2002).

**(iv) Talks and poster presentations**

1. **J. Tao** and Jian-Xin Zhu, Optical conductivity in strongly correlated electron materials, APS March Meeting in New Orleans, 2008.
2. **J. Tao**, I.V. Tokatly, and G. Vignale, Quantum Stress Focusing in Descriptive Chemistry, APS March Meeting in New Orleans, 2008.
3. **J. Tao**, Sergei Tretiak, and Jian-Xin Zhu, Excitation Energies from a ladder of time-dependent nonempirical density functionals, Conference on Excited State Processes in Electronic and Bio Nano-Materials, Santa Fe, New Mexico, October 1-4, 2007.
4. **J. Tao** and G. Vignale, Continuum Mechanics of an Inhomogeneous System, APS March Meeting in Denver, 2007.

5. **J. Tao** and G. Vignale, Time-Dependent Density Functional Theory beyond the Local Density Approximation, 52nd Midwest Solid State Conference in Kansas, Missouri, October 7-8, 2006.
6. **J. Tao** and G. Vignale, Dynamical Exchange-Correlation Potentials beyond the Local Density Approximation, APS March Meeting in Baltimore, 2006.
7. **J. Tao**, Nonempirical Construction of a Meta-GGA Density Functional and Extensions, 52nd Midwest Solid State Conference at Columbia, Missouri, October 8-9, 2005.
8. **J. Tao** and J. P. Perdew, Test of a Nonempirical Density Functional: Short-Range Part of the van der Waals Interaction in Rare-Gas Dimers, APS March Meeting in Los Angeles, 2005.
9. V.N. Staroverov, G.E. Scuseria, J.P. Perdew, **J. Tao**, and E.R. Davison, Comprehensive Assessment of a Nonempirical Density Functional, 228th ACS National Meeting in Philadelphia, August 22–26, 2004.
10. **J. Tao** and J. P. Perdew, New Meta-Generalized Gradient Approximation for the Exchange-Correlation, 225th ACS National Meeting in New Orleans, March 23–27, 2003.
11. **J. Tao** and J. P. Perdew, New Meta-Generalized Gradient Approximation for Exchange and Correlation in Austin, 2003.
12. **J. Tao** and J. P. Perdew, Construction of a New Meta-Generalized Gradient Approximation, workshop on DFT, Sandia National Laboratories in Albuquerque, New Mexico, August 16–18, 2002.
13. J. P. Perdew, **J. Tao**, and K. Schmidt, Nonempirical Meta- Generalized Gradient Approximation for Exchange, APS March Meeting in Seattle, 2001.
14. **J. Tao**, P. Gori-Giorgi, J. P. Perdew, and K. Schmidt, Correlation Energy Functional Compatible with Exact Exchange: Correlation Factor Model, APS March Meeting in Seattle, 2001.
15. P. Gori-Giorgi, **J. Tao**, and J. P. Perdew, Uniform Electron Gas from the Colle-Salvetti Functional: Missing Long-Range Correlations, APS March Meeting in Seattle, 2001.
16. K. Schmidt, S. Kurth, **J. Tao**, and J. P. Perdew, Remarks on a Model for the Correlation of the Uniform Electron Gas, APS March Meeting in Minneapolis, 2000.